DOE Operational User Requirements and Dispersion Modeling Capabilities

DOE Chemical & Biological Nonproliferation Program: Modeling and Prediction

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Department of Energy (DOE)

Workshop on
Multi-scale Atmospheric Dispersion Modeling
within the Federal Community

June 6–8, 2000

DOE Dispersion Modeling Operational Activities

- <u>Facility Safety Analysis</u>
  - Determine potential consequences of a facility before construction or modification; use during operation for risk assessment

- <u>Facility Emergency Preparedness and Response</u>
  - Develop hazard assessments, emergency action levels, and modeling systems to use in emergency response

- <u>Deployable Assets for Emergency Response (ARG, FRMAC, NEST, JTOT)</u>
  - Resources to protect public from major radiological accidents and terrorist events

- <u>Facility Annual Environmental Reporting</u>
  - Document exposure to public from routine operations

DOE Dispersion Modeling Operational Activities

Activity - Description	Authority or Requirement	Guidance	Dispersion Modeling Approach
Facility Safety Analysis	DOE Order 5480.23 (1997), NRC NUREG-1320 (1988) & CR-6410 (1998)	DOE-STD-1027-92 & 3009-94, DOE-HDBK-3010-94, NRC Reg. Guide 1.145 (1983), Accident Analysis Guidebook (2000), Accident Phenomenology & Consequence (APAC) Working Group Reports (1997-2000)	Graded approach – Model complexity commensurate with complexity or scale of effect, i.e., simple Gaussian to complex 3-D numerical codes
Facility Emergency Preparedness & Response	DOE Order 151.1 (1997, currently under revision)	DOE Guide 151.1 (1997, currently under revision), DOE Modeling Resources (1995)	Graded approach – Model complexity commensurate with complexity or scale of effect, i.e., simple Gaussian to complex 3-D numerical codes
Deployable Assets for Emergency Response (ARG, FRMAC, NEST, JTOT)	Federal Response Plan (FRP, 1995), Presidential Decision Directive 39 (PDD 39, 1995)	Federal Radiological Emergency Response Plan (FRERP, 1996), Overview of FRMAC Operations (2000), DoD Nuclear Weapons Accident Response Procedures (NARP, 1995)	Graded approach – Deployed teams use local models in the field and reach back to NARAC models
Facility Annual Environmental Reporting	DOE Orders 5400.1 & 231.1, CERCLA, SARA Title III, Natl. Emission Stds. for Haz. Air Pollutants (NESHAPS) 40 CFR 61	EPA Model Guideline	EPA annual model

DOE Dispersion Models Used Within DOE

Activity	Technical Forums	Dispersion Models Used
Facility Safety Analysis	DOE Energy Facility Contractors Group Safety Analysis Working Group (EFCOG SAWG) www.sawg2000.org	Radiological models: AI-RISK, AXAIR89Q, BNLGPM, COSYMA, ERAD, ETMOD, GENII, GXQ, HOTSPOT, MACCS2, MATHEW/ADPIC, PAVAN, RSAC 5, TRAC RA/HA, UFOTRI Chemical models: ADAM, ALOHA, CALPUFF, CASRAM, FEM3, HGSystem, INPUFF, SLAB, SCIPUFF, TSCREEN
Facility Emergency Preparedness & Response	DOE Emergency Management Issues Special Interest Group (EMI SIG) http://www.orau.gov/emi/ DOE Subcommittee on Consequence Assessment and Protective Actions (SCAPA) http://www.scapa.bnl.gov/	ALOHA (NOAA; National Safety Council) CAPARS (Hodgin, AlphaTrac) Epicode (Homann Associates) ERAD (Boughton, Sandia Natl Lab) HOTSPOT (Homann, LLNL) MDIF-VIS (NOAA ARL, INEEL) MIDAS (PLG) NARAC - ADAPT/LODI (Sugiyama & Nasstrom, LLNL) PGEMS (Allwine, PNNL) WINDS (Savannah River Lab)
Deployable Assets for Emergency Response (ARG, FRMAC, NEST, JTOT)	ARG, FRMAC, NEST, JTOT Working Groups http://www.dp.doe.gov/emergencyresponse/ http://www.nv.doe.gov/programs/frmac/	Local models used in the field: HOTSPOT, ERAD Reach back to NARAC models: ADAPT/LODI
Facility Annual Environmental Reporting	EPA SCRAM & Modeling Conferences http://www.epa.gov/scram001/	CAP-88

DOE Dispersion Modeling Capabilities Graded Approach

Hotspot Health Physics Codes

Deployed to emergency response personnel

SNL Atmospheric Dispersion and Consequence Prediction Capability

Deployed with expert atmospheric dispersion scientist

LLNL National Atmospheric Release Advisory Center (NARAC)

Reach-back to national center with expert assessment staff

Hotspot Health Physics Codes

- Purpose
  - To provide emergency response personnel and emergency planners with a fast, field-portable set of software tools for evaluating incidents involving radioactive material.
- Applications
  - Estimate the radiological impact following the release of radiological material from a continuous or puff release, explosive release, fuel fire or an area contamination event.
- Dispersion Model
  - A Gaussian plume/puff model with virtual source terms to model the initial atmospheric distribution of source material.
- Health Effects
  - Dose conversion factor library for inhalation, submersion and ground shine (ICRP-30 Library).

SNL Atmospheric Dispersion and Consequence Prediction Capability

- Purpose
  - Provide, on a field deployable system, predictions of the near field consequences which result from the dispersion of nuclear, chemical and biological releases

- Applications
  - Response to WMD terrorism incidents
  - Threat and safety analyses
  - Probabilistic risk assessments
  - Environmental impact statements

Steps in Prediction Process

- Characterize Source Term (Amount, Particle Size Distribution, Agent Viability, etc.) as a Function of Release Type
  - Explosive
  - Non-explosive aerosol
  - Fire-driven
  - Aerial
- Model Atmospheric Transport and Diffusion
- Estimate Dose and Health Effects
  - Toxicological models available for full range of chemical and biological agents and over 800 radionuclides

Steps in Prediction Process (cont'd)

- Develop Mitigation Strategy

- Communicate Results in a Format More Directly Useful to Decision Makers
  - Model predictions translated into health impacts
  - Results presented in an hierarchical format
    - Key results presented first
    - Additional details and supporting information available as needed
  - Non-expert able to "read" essential results quickly and unambiguously
  - Results for both unmitigated and mitigated release

AIRRAD Radionuclide Fallout Model

- **Model Description**
  - Implements methodology of DNA SIMFIC model
  - Square-root-of-time relationship for buoyant rise
  - Gaussian puff approach for turbulent dispersion
  - Workstation or PC compute platform

- **Capabilities**
  - Large number of hazard indicators
  - Graphical user interface
  - Full integration of model predictions with worldwide GIS

ERAD High Explosive Dispersal Model

- **Model Description**
  - Integral technique for source buoyancy
  - Probabilistic approach for turbulent dispersion
  - Parameterization of planetary boundary layer based on contemporary scaling theory
  - Workstation or PC compute platform

- **Capabilities**
  - Gaseous and particle sources
  - Treats penetration of elevated inversions
  - Graphical user interface
  - Full integration of model predictions with worldwide GIS

National Atmospheric Release Advisory Center

- NARAC's *mission* is to provide timely and credible asessment advisories to emergency managers for nuclear and other hazard releases to the atmosphere and thereby minimize the exposure of the population at risk.

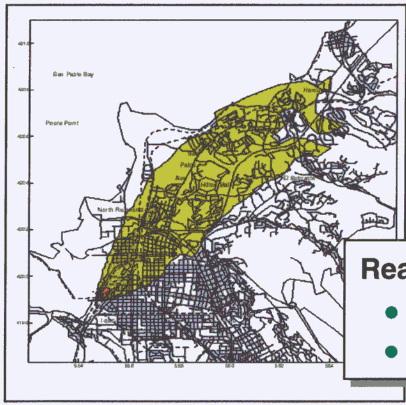
- The mission requirements apply worldwide wherever and whenever DOE and DoD Emergency Planning and Response programs have a requirement or our government deems there is an event of interest.

National Atmospheric Release Advisory Center (NARAC)

Real-time advisories for hazardous atmospheric releases

World-wide coverage
- Terrain & land-surface
- Vector & raster maps
- Real-time weather data

National Center at LLNL
- Expert assessment staff
- Advanced modeling system

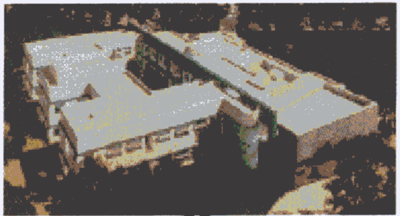


Real-time Hazard Advisories
- Available within minutes
- Distributed electronically

NARAC staff operates the center, trains users and deploys for special events

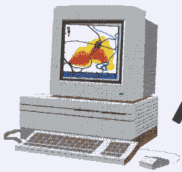
Access to the National Atmospheric Release Advisory Center (NARAC)

National Center in Livermore

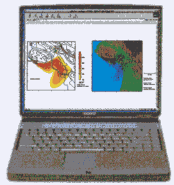


Dedicated Intranet
or Dial-up

Communication links using
Internet protocols (Internet
intranet, dial-up, wireless)

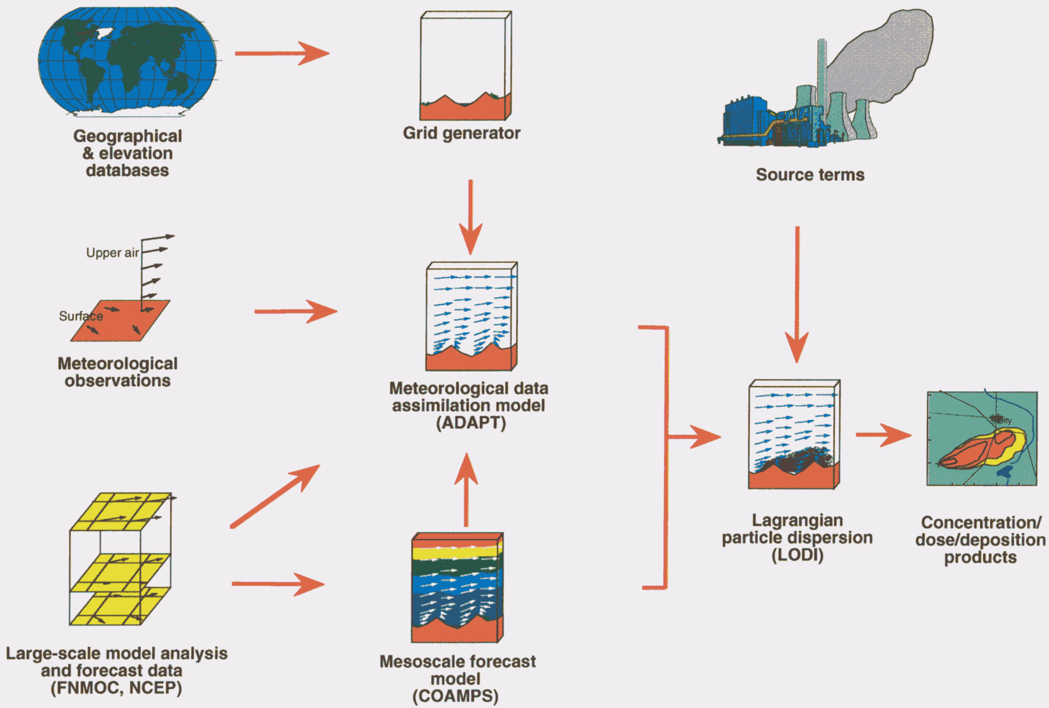


**Site Workstation System (SWS)
at DOE/DoD Facilities**



**Internet Remote Access (IRA) System
for Local EOC or
Deployment to Remote Site
(Under Development)**

NARAC Modeling System



NARAC Weather Forecast Model (COAMPS)

- **COAMPS** - Naval Research Laboratory model (Hodur, 1996)
- **Grids**
  - Arakawa-C grid, continuous terrain representation, vertical coordinate
  - Multiple nested grids
- **Data analysis and initialization**
  - Multivariate optimum interpolation analysis of winds and temperature
  - Time-dependent boundary conditions (Davies, QJRMS 1976; Perkey and Krietzberg, MWR 1976)
- **Dynamics**
  - Non-hydrostatic compressible (Klemp and Wilhelmson, JAS 1978)
  - 2nd order advection, 4th order diffusion
- **Atmospheric physics**
  - Radiation (Harshvardhan, JGR 1987)
  - Explicit moist physics (Rutledge and Hobbs, JAS 1983)
  - Convective precipitation physics (Kain and Fritsch, JAS 1990; Kuo, JAS 1979)
  - Boundary layer physics (Mellor and Yamada, 1982)
  - Surface layer physics (Louis, 1979)

NARAC Meteorological Data Assimilation Model (ADAPT)

- **Grids**
  - Variable-resolution grids
  - Continuous terrain representation, σ_z vertical coordinate
  - Map projection for multiple scales
- **Assimilation of meteorological and land-surface data**
  - Observational data (e.g, surface, tower, profiler, rawinsonde)
  - Weather forecast model data (e.g, AVN, COAMPS, NOGAPS, ETA)
  - Land-surface data (e.g, z_0, d, land use category)
- **Interpolation and parameterization**
  - Multiple interpolation algorithms
  - Vertical parameterization options
- **Meteorological variables**
  - Non-divergent wind field ($\nabla \cdot V = 0$) based on variational principal and finite-element spatial discretization and conjugate gradient solution method
  - Temperature, pressure, humidity, and other scalar fields
  - Precipitation
  - Diagnostic eddy diffusivity parameterization based on scaling relationships
  - Turbulence scaling parameters derived from land-surface and surface meteorological data

NARAC Dispersion Model (LODI)

- Lagrangian stochastic (Monte Carlo) diffusion method
- Nested meteorological data grids
- Variable-resolution concentration and deposition grids
- Multiple, moving receptors
- Point, line, area, and Gaussian sources
- Aerosol mass-size distributions (log-normal or table)
- Multiple, moving, time-varying sources
- Momentum and buoyancy plume rise
- Decay and production of radionuclides in decay chains
- First-order decay of biological and chemical material
- Dry deposition (from gravitational settling velocity and deposition resistance)
- Precipitation scavenging (from aerosol size and precipitation rate)

NARAC Model Testing and Evaluation

- **Model evaluation**
  - Testing of individual models
  - Comparisons with known analytic solutions
  - Component testing of individual physical processes and numerics
- **Laboratory experiments**
  - Comparisons with wind/water tank experimental results
- **Field experiment case studies (ADAPT/LODI)**
  - Project Prairie Grass: Flat terrain; continuous near-surface point source of SO_2; 50-800 meter downwind distance
  - Savannah River Mesoscale Atmospheric Tracer Studies (MATS) : Rolling, tree-covered terrain; 15-min SF_6 release at 61 meters; 30 km range
  - Diablo Canyon Tracer Study (DOPPTEX) : Hilly, coastal terrain; continuous and pulsating SF_6 releases at surface and 71m; 1-40 km range
  - European Tracer Experiment (ETEX) : Continental Europe, and U.K; 12-hr continuous perfluorocarbon tracer gas release near surface; 20-2000 km
- **Operational testing**
  - Performance and speed
  - Robustness
  - Default model input settings

DOE - DTRA (DoD) Model Intercomparison Project

- **Purpose**
  - Collaborative effort to advance the atmospheric hazard assessment prediction capabilities of both the DOE and DoD through a scientifically based joint modeling system evaluation and comparison study
- **Plan**
  - Develop a joint understanding of the DOE and DoD modeling systems
  - Evaluate the modeling systems for an initial set of experimental data sets and a variety of conditions (meteorology, land-surface, turbulence, source)
  - Distinguish variations due to model physics and numerics from differences due to operational default choices
- **Comparison Metrics**
  - Statistical criteria: spatially/temporally paired point-to-point statistical comparisons of model output and measured concentration values (ratio factors, normalized mean square error, bias, etc.)
  - Graphical criteria: overlays of measured values and model contours
- **Initial Case Studies (FY00)**
  - Dispersion model-to-model comparisons for simple scenarios
  - Project Prairie Grass (microscale experiment, 1956)
  - Dugway Phase 1 (DoD microscale puff dispersion experiment, 1996)

DOE CBNP
Modeling and Prediction

Chem-Bio Transport and Fate in Urban Environments

Argonne National Laboratory
Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Pacific Northwest National Laboratory
Sandia National Laboratories

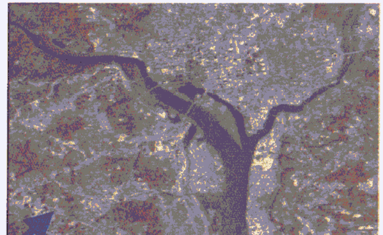
Department of Energy
Chemical & Biological Nonproliferation Program

Goal
Modeling and Prediction

Building Interiors

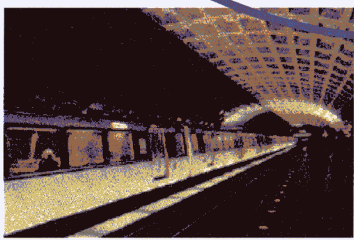
"...to accurately predict the dispersion and ultimate fate of chemical and biological agents released into the urban environment..."

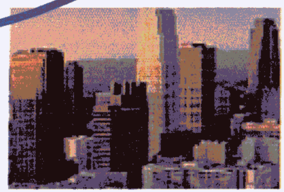
Urban-Regional



Subway

Multiple Interacting Scales





Exterior Building

Counterterrorism Incident Response in
Urban Areas and at Special Events

Multi-Scale Transport Models

- COMIS Multizone Building Interiors Model
- STAR-CD Building Interior CFD Model
- SES Subway System Model
- FEM3CB Exterior Building Scale CFD Model
- HIGRAD Exterior Many Building CFD Model
- COAMPS/LODI Exterior Parameterized Urban-Regional Model

Building Scale Airflow and Dispersion Model (FEM3CB)

- Computational Fluid Dynamics (CFD) code based on the finite element approach
- Flexible grid system capability including variable resolution, distorted meshes and explicit representation of terrain
- Capability of resolving individual buildings in great detail or few buildings at varying resolutions
- Runs on ASCI's massively parallel platforms
- Current model physics:
  - Neutral or heavier-than-air (chemical) agents
  - Aerosol physics (biological agents)
  - Surface heating and shading
  - Tree canopy parameterization
  - Reynolds-averaged (RANS) and Large Eddy Simulation (LES) turbulence models
  - First order UV degradation submodel

Salt Lake City
Fall 2000 Field Experiments

- **Single Building (SF6) [CBNP]**
  - 2 to 4 hour experiments
  - Instantaneous line source outside building (>1 ppm SF6)
  - 45 Tracer samplers located inside and outside building (15 bags–programmable)
  - 5 to 10 minute sampling times in bags
  - 6 Fast-response SF6 instruments (1 Hz data)
  - 6 Sonic anemometers (10 Hz data)
  - 1 Open-path FTIR for SF6 mapping
- **Multi-Building to Urban-Scale (SF6–PFT) [CBNP/VTMX]**
  - 12 to 18 hour experiments
  - 1 2 to 3 hour PFT point release at single building
  - 1 6 to 8 hour PFT point release downtown
  - 40 Tracer samplers (12 bags/CATS tubes–programmable)
  - 15 minute to 1 hour sampling in bags/CATS
  - 24 Temperatures loggers for urban temperature mapping
  - 3 Surface weather stations
- **Urban-Scale to Mesoscale (PFT) [VTMX]**
  - 12 to 18 hour experiments
  - 2 6 to 8 hour PFT point releases outside of downtown
  - 60 PFT samplers (23 tubes–programmable)
  - 1 to 3 hour PFT sampling in tubes
  - 6 Radar profilers (with RASS)
  - 4 Sodars
  - 3 Tethersonde systems
  - 1 Doppler lidar
  - 3 Rawinsonde systems
  - 6 3-D sonics for fluxes
  - 10 Surface weather stations
  - NWS rawinsondes